Table S9: Projections of simulations onto 2D-surface using two PC1 modes from unperturbed unbound and bound states. Unbound (green) and bound (brown) states are plotted on the same surface for comparison. Index indicates the residue being held rigid.

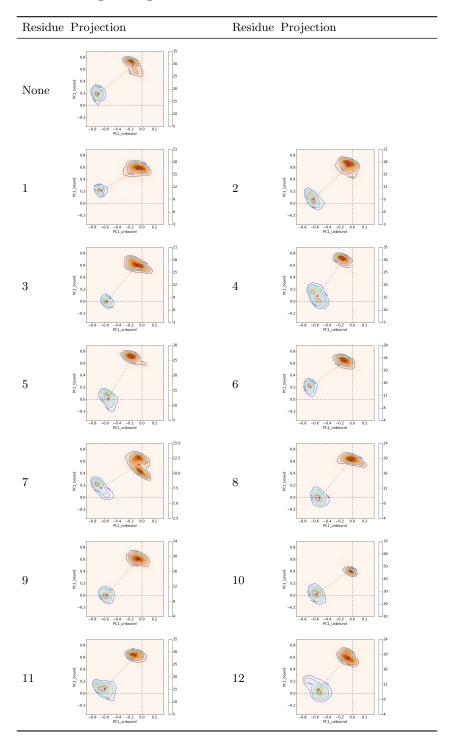


Table S9: Projections of simulations onto 2D-surface using two PC1 modes from unperturbed unbound and bound states. Unbound (green) and bound (brown) states are plotted on the same surface for comparison. Index indicates the residue being held rigid.

Residue	e Projection	Residue	Projection
13	0.8 0.6 0.6 0.7 0.7 0.9 0.2 0.0 0.2 0.5 0.2 0.5 0.2 0.5 0.2 0.0 0.5 0.2 0.0 0.2 0.5 0.2 0.0 0.5 0.2 0.0 0.2 0.5 0.2 0.0 0.5 0.2 0.0 0.0	14	0.8 0.6 0.0 0.2 0.0 0.0
15	0.8 0.6 0.6 0.6 0.6 0.6 0.2 0.0 0.0	16	0.0 56 0.0 6 0.0 0.0 0.0 0.0 0.0 0.0 0.0 0.0
17	0.8 0.6 0.6 0.6 0.6 0.0 0.2 0.0 0.0	18	0.8 0.4 20 16 16 12 0.0 0.0 0.2 0.0 0.2 0.0 0.2 0.0 0.2 0.0 0.2 0.0 0.2 0.0 0.2 0.0 0.2 0.0 0.2 0.0 0.2 0.0 0.2 0.0 0.2 0.0 0.0
19	0.8 0.6 0.6 0.6 0.2 0.0 0.2 0.0 0.2 0.5 0.2 0.5 0.2 0.5 0.2 0.5 0.5 0.5 0.5 0.5 0.5 0.5 0.5 0.5 0.5	20	0.6 0.6 0.6 0.0 0.2 0.0 0.0
21	0.8	22	0.0 0.0 1.0 1.0 1.0 1.0 1.0 1.0 1.0 1.0
23	0.8 0.6 0.6 0.4 0.2 0.0 0.0	24	0.8 0.6 0.6 0.0 0.2 0.0 0.2 0.0 0.2 0.4 0.2 0.0 0.2 0.4 0.4 0.2 0.0 0.2 0.0 0.2 0.4 0.2 0.0 0.2 0.0 0.2 0.0 0.2 0.0 0.2 0.0 0.0
25	0.8 0.6 0.6 0.6 0.6 0.6 0.6 0.6 0.6 0.6 0.6	26	0.8 0.4 0.2 0.0 0.2 0.0 0.2 0.5 0.5 0.5 0.5 0.5 0.5 0.5 0.5 0.5 0.5

Table S9: Projections of simulations onto 2D-surface using two PC1 modes from unperturbed unbound and bound states. Unbound (green) and bound (brown) states are plotted on the same surface for comparison. Index indicates the residue being held rigid.

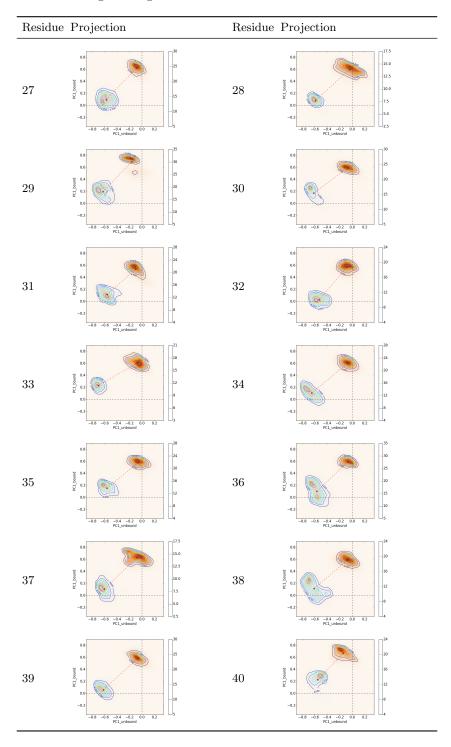


Table S9: Projections of simulations onto 2D-surface using two PC1 modes from unperturbed unbound and bound states. Unbound (green) and bound (brown) states are plotted on the same surface for comparison. Index indicates the residue being held rigid.

Residue	e Projection	Residue	Projection
41	0.8 0.8 0.4 0.2 0.0 0.0	42	0.0 0.0 0.0 0.0 0.0 0.0 0.0 0.0 0.0 0.0
43	0.8 0.6 0.6 0.6 0.0 0.2 0.0 0.2 0.5 0.2 0.0 0.2 0.5 0.5 0.5 0.5 0.5 0.5 0.5 0.5 0.5 0.5	44	0.8 0.6 0.4 0.2 0.0 0.2 0.3 0.3 0.3 0.2 0.3 0.3 0.3 0.3 0.3 0.3 0.3 0.3 0.3 0.3
45	0.8 0.6 0.6 0.6 0.6 0.0 0.0 0.0 0.0 0.0 0.0	46	0.0 0.0 17.5 15.0 12.5 10.0 0.0 12.5 10.0 12.5
47	0.8 0.6 0.6 0.6 0.2 0.0 0.2 0.5 0.2 0.5 0.2 0.5 0.2 0.0 0.2 0.0 0.2 0.0 0.2 0.0 0.2 0.0 0.2 0.0 0.2 0.0 0.2 0.0 0.2 0.0 0.2 0.0 0.0	48	0.0 0.0 0.0 0.0 0.0 0.0 0.0 0.0 0.0 0.0
49	0.8	50	0.6 0.6 0.4 0.2 0.6 0.2 0.5 0.2 0.5 0.5 0.5 0.5 0.5 0.5 0.5 0.5 0.5 0.5
51	0.6 0.6 0.6 0.6 0.6 0.6 0.6 0.6 0.6 0.6	52	0.6 0.6 0.6 0.6 0.2 0.0 0.2 0.5 0.5 0.5 0.5 0.5 0.5 0.5 0.5 0.5 0.5
53	0.6 0.6 0.6 0.6 0.0 0.2 0.0 0.2 0.5 0.5 0.5 0.5 0.5 0.5 0.5 0.5 0.5 0.5	54	0.8 0.4 1.5 1.5 1.2 9 0.4 0.2 0.0 0.2 0.3 1.5 1.5 1.2 1.2 1.8 1.5 1.5 1.2 1.2 1.8 1.5 1.5 1.2 1.2 1.8 1.5 1.5 1.2 1.2 1.3 1.5 1.5 1.2 1.5 1.5 1.5 1.5 1.5 1.5 1.5 1.5 1.5 1.5

Table S9: Projections of simulations onto 2D-surface using two PC1 modes from unperturbed unbound and bound states. Unbound (green) and bound (brown) states are plotted on the same surface for comparison. Index indicates the residue being held rigid.

Residue	Projection	Residue	Projection
55	0.6 0.6 0.6 0.6 0.6 0.6 0.6 0.6 0.6 0.6	56	0.0 0.0 12.5 10.
57	0.8 0.6 0.6 0.6 0.6 0.6 0.6 0.6 0.6 0.6 0.6	58	0.6 0.6 0.6 0.6 0.6 0.6 0.0 0.2 0.5 0.5 0.5 0.5 0.5 0.5 0.5 0.5 0.5 0.5
59	0.8 0.6 0.6 0.4 0.2 0.0 0.2 0.5 0.5 PCI, unbound	60	0.8 0.6 0.6 0.6 0.6 0.0 0.2 0.0 0.2 0.5 0.5 0.6 0.6 0.6 0.7 0.2 0.0 0.2 0.5 0.5 0.5 0.5 0.5 0.5 0.5 0.5 0.5 0.5
61	0.6 0.6 0.6 0.6 0.6 0.6 0.6 0.6 0.6 0.6	62	0.6 0.6 0.6 0.6 0.2 0.5 0.5 0.5 0.5 0.5 0.5 0.5 0.5 0.5 0.5
63	0.6 0.6 0.6 0.6 0.6 0.6 0.6 0.6 0.6 0.6	64	0.6 0.6 0.6 0.6 0.6 0.2 0.6 0.2 0.6 0.2 0.6 0.2 0.6 0.2 0.6 0.2 0.6 0.2 0.6 0.2 0.6 0.2 0.6 0.2 0.6 0.2 0.6 0.2 0.6 0.2 0.6 0.6 0.2 0.2 0.2 0.2 0.2 0.2 0.2 0.2 0.2 0.2
65	0.8 0.6 0.6 0.6 0.6 0.0 0.2 0.0 0.2 0.5 0.0 0.2 0.5 0.5 0.0 0.2 0.5 0.5 0.5 0.5 0.5 0.5 0.5 0.5 0.5 0.5	66	0.8 0.4 0.2 0.0 0.2 0.0 0.2 0.3 0.0 0.2 0.3 0.0 0.2 0.3 0.0 0.0 0.2 0.0 0.3 0.0 0.0 0.2 0.0 0.0 0.2 0.0 0.0 0.0 0.0
67	0.6 0.6 0.6 0.6 0.6 0.6 0.6 0.6 0.6 0.6	68	0.8 0.0 0.0 0.0 0.0 0.0 0.0 0.0 0.0 0.0

Table S9: Projections of simulations onto 2D-surface using two PC1 modes from unperturbed unbound and bound states. Unbound (green) and bound (brown) states are plotted on the same surface for comparison. Index indicates the residue being held rigid.

Residue	e Projection	Residue	Projection
69	0.8 0.6 0.6 0.6 0.6 0.6 0.6 0.6 0.6 0.6 0.6	70	0.8 0.6 0.6 0.4 0.2 0.9 0.2 0.4 4
71	0.8 0.6 0.6 0.4 0.2 0.0 0.2 0.2 0.2 0.2 0.2 0.2 0.2 0.2	72	0.0 0.0 0.0 0.0 0.0 0.0 0.0 0.0 0.0 0.0
73	0.6 0.6 0.6 0.6 0.0 0.0 0.2 0.0 0.2 0.0 0.2 0.0 0.2 0.0 0.2 0.0 0.2 0.0 0.2 0.0 0.2 0.0 0.2 0.0 0.2 0.0 0.2 0.0 0.2 0.0 0.2 0.0 0.0	74	0.8 0.4 1.5 1.5 1.5 1.2 1.2 1.8 0.6 0.6 0.6 0.4 0.2 0.0 0.2 0.5 0.5 1.5 1.5 1.2 1.2 1.2 1.2 1.3 1.5 1.5 1.2 1.2 1.2 1.3 1.3 1.5 1.5 1.5 1.5 1.5 1.5 1.5 1.5 1.5 1.5
75	0.8 0.6 0.6 0.6 0.6 0.7 0.7 0.7 0.8 0.8 0.8 0.8 0.8 0.8 0.8 0.8 0.8 0.8	76	0.0 0.0 12 12 12 12 12 12 12 12 12 12 12 12 12
77	0.8 0.4 0.5 0.5 0.5 0.5 0.5 0.5 0.5 0.5 0.5 0.5	78	0.6 0.6 0.6 0.4 0.2 0.6 0.2 0.2 0.6 0.2 0.2 0.2 0.2 0.2 0.2 0.2 0.2 0.2 0.2
79	0.8 0.6 0.6 0.6 0.6 0.6 0.6 0.6 0.6 0.6 0.6	80	0.6 0.6 0.6 0.6 0.2 0.0 0.2 0.4 0.2 0.4 0.2 0.4 0.4 0.2 0.4 0.4 0.4 0.4 0.4 0.4 0.4 0.4 0.4 0.4
81	0.6	82	0.8 0.4 0.2 0.0 0.2 0.2 0.0 0.2 0.0 0.2 0.0 0.2 0.0 0.2 0.0 0.2 0.0 0.2 0.0 0.2 0.0 0.2 0.0 0.0

Table S9: Projections of simulations onto 2D-surface using two PC1 modes from unperturbed unbound and bound states. Unbound (green) and bound (brown) states are plotted on the same surface for comparison. Index indicates the residue being held rigid.

